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United States Environmental Protection Agency  
Washington, DC 20460

*E. White*

**ORIGINAL**

Document Description

**SAT L-07-299**

Date

**7/20/07**

**STRUCTURE ACTIVITY TEAM REPORT**

ver. 04/98

Case #: L-07-0299

DCN:

SAT Date: 6/29/2007

SAT Chair: V. Nabholz

Submitter: Tracerco

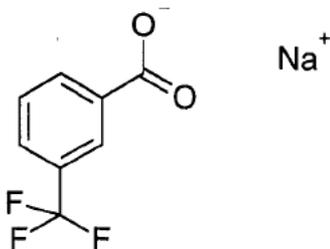
Chemical Name:

Benzoic acid, 3-(trifluoromethyl)-, sodium salt (1:1)

CAS RN: 62996-41-1

Trade Name: Tracerco 190t

**Structure**



Molecular Formula:  $C_8H_4F_3NaO_2$

Molecular Wt. 212

WT% < 500:

WT% < 1000:

MP:

BP:

Eq. Wt:

H2O Sol (g/L): >200 V.P. <0.000001

Max. Prod. Volume (kg/yr): 700 Physical State: Solid (cream powder)

USE:

Tracer chemical to measure flow in deep oil-bearing strata.  
 STN file CA: 3 references found, describing its properties and use as a chemical intermediate.  
 Similar cases concurrently submitted: L-07-0298, L-07-0300.  
 P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

FOCUS Date: JUL 19 2007

Results: *Conditional Grant* P2REC → CCU

STRUCTURE ACTIVITY TEAM REPORT 29 June 2007

CASE NUMBERS: L07-0290 to L07-<sup>300</sup>~~0330~~

L07-0290 (F2)  
L07-0291 (F)  
L07-0292 (F2)  
L07-0293 (F2)  
L07-0294 (F2)  
L07-0295 (F2)  
L07-0296 (F4)  
L07-0297 (F3)  
L07-0298 (CF3)  
L07-0299 (CF3)  
L07-0300 (CF3)

P2REC: substitute for radionuclide tracers

RELATED CASES:

L07-0271 (F)

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	<u>HEALTH</u>	<u>ECOTOX</u>
LEVEL:	1-2	1

KEYWORDS: DEVEL, LIVER, KIDNEY, SENS-ASTHMA, MUTA

SUMMARY OF ASSESSMENT:

FATE: MW162 to 216  
solids with mp for L070271 (F) = 126 °C (M)  
log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI),  
1.59 to 3.10 (M)  
log Kow for L070271 = -5.87 with pH? (HPLC)  
log Kow for L070296 = -2.11 with pH? (HPLC)  
log Kow for L070297 = -3.62 with pH? (HPLC)  
log Kow for L070298 = -1.64 with pH? (HPLC)  
S > 200 mg/L to > 10 g/L at 20 °C (P)  
vp < 1.0E-6 mm Hg or torr at 25 °C (P)  
bp = 460 °C (P)  
H for the covalent ion pair = 1.2E-7 to 9.5E-7 (P)  
log Koc for the covalent ion pair = 1.4 to 2.0 (P)  
log fish BCF = 0.50 (P)  
sorption to sludge = low (P)

test data for L070271 for aerobic biodegradation in seawater at 20 C, via closed bottle (OECD306) were:

time (d)	biodegradation (percent)
5	0
14	2
28	63

test data for aerobic biodegradation for the [REDACTED] [REDACTED] of L070299 from [REDACTED] were:  
15% biodegradation in 28 d, thus, not readily biodegradable via CO2 evolution in modified Sturm test (OECD301B); if test result is due solely to ester hydrolysis and degradation of the [REDACTED] moiety, then removal via POTW of the parent would be  $\geq 90\%$  but notifier did not measure degradation products;

POTW removal = 0% to 90 via sorption and possible biodegradation  
time for complete ultimate aerobic biodegradation = weeks to  $\Rightarrow$  months

sorption to soils and sediments = low (P)

PBT Potential: P2B1T2 to P3B1T2

\*CEB FATE: migration to ground water = rapid

HEALTH: Absorption nil thru skin based on physical/chemical properties; good thru lungs based on analogs; and good thru the GI tract based on analogs;

test data for the [REDACTED] [REDACTED] of L070299, [REDACTED] were:  
rat acute oral LD50 = 800 mg/kg with toxic signs; LD100 = 2 g/kg, LD0 = 300 mg/kg;  
rat acute dermal LD0 = 2.0 g/kg with no toxic signs;  
slight and transient (2 d) skin irritation in rabbits;  
slight and transient (1 d) eye irritation in rabbits;  
Ames test was negative;  
E. coli test was negative;  
chromosome aberration test with V79 cells was positive with activation, but negative without activation;  
no skin sensitization in guinea pigs (M&K);  
rat 28-d subchronic oral-gavage with doses = 1000, 300, and 100 mg/kg/d with NOAEL = 100 mg/kg/d and LOEL = 300 mg/kg/d based on salivation and increased water consumption; effects at 1000 mg/kg/d were slight to severe salivation, unsteady gait, motor activity significantly decreased and effects to the liver and kidneys;

concern for asthma and developmental toxicity based on data for benzoic acid, note: the mechanism for the asthma is unknown;

concern for possible mutagenicity, liver toxicity, and kidney toxicity based on data for [REDACTED] which was the [REDACTED] [REDACTED] of L070299, however, the [REDACTED] will have some acylating activity

which is absent in the acid, thus, the acid will be less toxic than the [REDACTED] [REDACTED]

low to moderate concern for toxicity

\*CEB HEALTH: Exposures to humans: inhalation, ingestion, and drinking water;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	>	100.0	P
SW fish 96-h LC50	=	440.0	M S,N L070271
SW fish 96-h LC50	>	320.0	M S,N L070290
SW fish 96-h LC50	>	320.0	M S,N L070291
daphnid 48-h LC50	>	100.0	P
SW invert Ac ton 48-h LC50	=	2830.0	M S,N L070271
SW invert Ac ton 48-h LC50	=	1500.0	M S,N L070290
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070291
SW invert Ac ton 48-h LC50	=	480.0	M S,N L070292
SW invert Ac ton 48-h LC50	=	270.0	M S,N L070293
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070294
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070295
SW invert Ac ton 48-h LC50	=	300.0	M S,N L070296
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070297
SW invert Ac ton 48-h LC50	=	440.0	M S,N L070298
SW invert Ac ton 48-h LC50	=	170.0	M S,N L070299
SW invert Ac ton 48-h LC50	=	130.0	M S,N L070300
green algal 96-h EC50	>	100.0	P
SW algae Sk cost 72-h EC50 c	=	250.0	M S,N L070271
SW algae Sk cost 72-h EC50 r	>	10000.0	M S,N L070290
SW algae Sk cost 72-h EC50 r	=	430.0	M S,N L070291
SW algae Sk cost 72-h EC50 r	=	660.0	M S,N L070292
SW algae Sk cost 72-h EC50 r	=	2100.0	M S,N L070296
SW algae Sk cost 72-h EC50 r	=	1500.0	M S,N L070297
SW algae Sk cost 72-h EC50 r	=	700.0	M S,N L070300
fish chronic value	>	10.0	P
daphnid ChV	>	10.0	P
algal ChV	>	10.0	P
SW algae Sk cost ChV c	=	100.0	M S,N L070271
SW algae Sk cost ChV r	=	5600.0	M S,N L070290
SW algae Sk cost ChV r	<	100.0	M S,N L070291
SW algae Sk cost ChV r	=	320.0	M S,N L070292
SW algae Sk cost ChV r	=	1000.0	M S,N L070296
SW algae Sk cost ChV r	=	320.0	M S,N L070297
SW algae Sk cost ChV r	=	320.0	M S,N L070300
benthic			
SW invert Coror vol 10-d LC50	=	6558.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d NOEC	=	470.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d LC50	=	7300.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d LC50	=	3800.0	mg/kg DWT M S,N L070291
SW invert Coror vol 10-d NOEC	=	150.0	mg/kg DWT M S,N L070291

SW invert Coror vol 10-d LC50	=	6700.0	mg/kg	DWT M S,N	L070292
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg	DWT M S,N	L070292
SW invert Coror vol 10-d LC50	=	410.0	mg/kg	DWT M S,N	L070296
SW invert Coror vol 10-d NOEC	=	130.0	mg/kg	DWT M S,N	L070296
SW invert Coror vol 10-d LC50	=	330.0	mg/kg	DWT M S,N	L070297
SW invert Coror vol 10-d NOEC	=	160.0	mg/kg	DWT M S,N	L070297
SW invert Coror vol 10-d LC50	=	280.0	mg/kg	DWT M S,N	L070300
SW invert Coror vol 10-d NOEC	=	16.0	mg/kg	DWT M S,N	L070300

Predictions are based on SARs for neutral organic chemicals with 10X less toxicity due to the substitution of the acid, or SARs for anionic surfactants-carboxylic acid-C4.Na; SAR chemical class = surfactant-anionic-F1 to F4 and CF3 benzene-COO.Na; MW162 to 216; solids with mp for L070271 (F) = 126 °C (M); log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI), 1.59 to 3.10 (M); log Kow for L070271 = -5.87 with pH? (HPLC); S > 200 mg/L at 20 °C (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L; low concern for toxicity

assessment factor = 10.0  
concern concentration = 1.0 mg/L (ppm)  
\*CEB ECOTOX: No releases to water;

P2REC: forward to FOCUS with support.

SAT Co-chair: Vince Nabholz, 564.8909

# GTOX Report

PMN No.  
**L-07-0299**

CAS No.  
**069226-41-1**

Rcvd:  
**06/18/07**

OECD  
**Incomplet**

ID: Rec# 4 : 863

S/A  
**S**

Name of Analog

Reviewer  
**KED**

with activation

without activation

Positive Strains

Salmonella Assay:

Chromosomal Aberration

CHO:

CHL:

V79:

E. coli Reverse Mutation:

Mouse Micronucleus Assay:

Route:

Rat Hepatocytes Unscheduled DNA Synthesis:

Other GTOX Results

Comments

ECOTOX:

Fate:

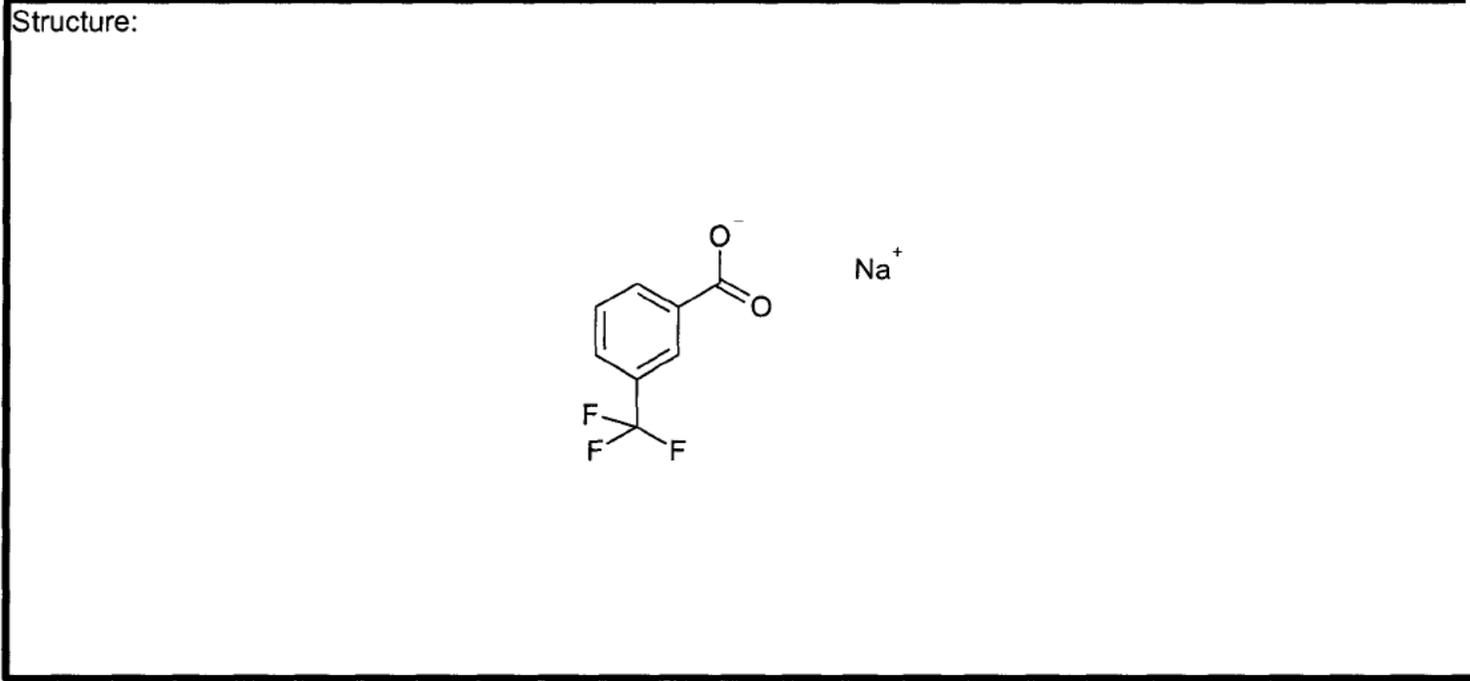
WS/Log P:

NCSAB SAT REPORT

(N):

PMN: L-07-0299 CAS RN: 62996-41-

Chemical Name: Benzoic acid, 3-(trifluoromethyl)-, sodium salt (1:1)  
 Analogs:  
 Production Volume: 700.0



Use: Super chemical to measure flow in deep oil-bearing strata.  
 STN file CA: 3 references found, describing its properties and use as a chemical intermediate.  
 Similar cases concurrently submitted: L-07-0298, L-07-0300.  
 P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata.

Formula:  $C_8H_4F_3NaO_2$  Eq Wt:

Mol Weight: 212.10 Wt% < 500: Wt% < 1000:

MP: BP: VP: < 0.000001

H2O Sol (g/L): > 200 Physical State: Solid (cream powder) Log P:

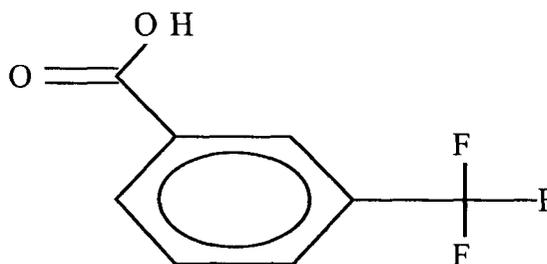
Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h			
Daphnid 48-h			
Algal 96-h			
Fish ChV			
Daphnid ChV			
Algal ChV			
BCF			

CHEMICAL CLASS: SAR:

ECOTOX CONCERN H M L CONCERN CONCENTRATION

DATE ASSESSOR:

L-07-299



SMILES : FC(F)(F)c1cccc(c1)C(=O)O  
 CHEM :  
 CAS Num:  
 ChemID1:  
 ChemID2:  
 ChemID3:  
 MOL FOR: C8 H5 F3 O2  
 MOL WT : 190.12  
 Log Kow: 2.94 (User entered)  
 Melt Pt: 106.00 deg C  
 Wat Sol: 57.78 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

-----  
 Neutral Organics-acid

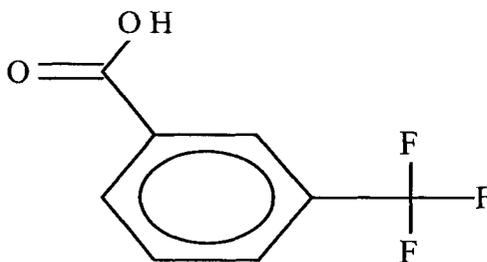
ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	38.752

--> Acid moiety found: Predicted values multiplied by 10

Neutral Organics-acid	: Fish	96-hr	LC50	184.261 *
Neutral Organics-acid	: Fish	14-day	LC50	387.520 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	210.685 *
Neutral Organics-acid	: Green Algae	96-hr	EC50	139.038 *
Neutral Organics-acid	: Fish	30-day	ChV	27.621
Neutral Organics-acid	: Daphnid	16-day	EC50	16.302
Neutral Organics-acid	: Green Algae	96-hr	ChV	23.937
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	66.502 *
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	27.167

				mg/kg (ppm) dry wt soil =====
Neutral Organics-acid	: Earthworm	14-day	LC50	6005.016 *

Note: \* = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.  
 Fish and daphnid acute toxicity log Kow cutoff: 5.0  
 Green algal EC50 toxicity log Kow cutoff: 6.4  
 Chronic toxicity log Kow cutoff: 8.0  
 MW cutoff: 1000



SMILES : FC(F)(F)c1cccc(c1)C(=O)O  
 CHEM :  
 MOL FOR: C8 H5 F3 O2  
 MOL WT : 190.12

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L):	-----	Log Kow (oct-water):	2.94
Vapor Pressure (mm Hg):	-----	Boiling Pt (deg C):	-----
Henry LC (atm-m3/mole):	-----	Melting Pt (deg C):	106.00

Log Kow (KOWWIN v1.67 estimate) = 2.84 Exp database: 2.95

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C):	254.62	BP(exp database):	238.5 deg C
Melting Pt (deg C):	60.17	MP(exp database):	105.5 deg C
VP(mm Hg,25 deg C):	0.00771		

Water Solubility estimate (WSKOW v1.41): 507.5 mg/L

Water Solubility estimate (fragments): 43.256 mg/L

Henrys Law Constant (atm-m3/mole) [HENRYWIN v3.10]:

Bond Method: 9.42E-007 Group Method: Incomplete  
 Henrys LC [VP/WSol estimate using EPI values]: 3.800E-006 atm-m3/mole

Biodegradation Estimates (BIOWIN v4.02):

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

OH Half-Life = 16.081 Days (12-hr day; 1.5E6 OH/cm3)  
 No Ozone Reaction Estimation

Soil Adsorption (PCKOCWIN v1.66): Koc = 103.4 Log Koc = 2.015

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF estimate (BCFWIN v2.15): Log BCF = 0.500 (BCF = 3.162)

Volatilization from Water: (Henry LC = 9.42e-007 atm-m3/mole)

Half-Lives: Model River = 858.4 hr, Model Lake = 9480 hr

Removal In Wastewater Treatment (percents,99% recommended maximum):

TOTAL: 5.26, Biodeg: 0.12, Sludge: 5.09, Air: 0.05

Level III Fugacity Model (conc %,half-life hr):

Air(1.92%,386),Water(18%,900),Soil(79.7%,1.8e+003),Sediment(0.36%,8.1e+003)  
 Persistence Time: 1.17e+003 hr

CHEMICAL: Unknown

10:52:18 06/27/:7

MOL WT : 190.13

MOL FOR: C8H5F3O2

SMILES : FC(F)(F)c1cccc(c1)C(O)=O

ISOC-ID: -----a-aaaa-a-----

FRAG-ID: 11 1 1 2 2 2

H-COUNT: 111 1 1

Class	Type	Contribution Description	Comment	Value
FRAGMENT	# 1	Trifloromethyl-	MEASURED	1.110
FRAGMENT	# 2	Carboxy (Zw-)	MEASURED	-0.030
ISOLATING	CARBON	6 Aromatic isolating carbon(s)		0.780
EXFRAGMENT	HYDROG	4 Hydrogen(s) on isolating carbons		0.908
ELECTRONIC	SIGRHO	1 Potential interactions; 1.00 used	withinRing	0.172
RESULT	v3.3	All fragments measured	ESTIMATE	2.940

ATTENDEES

SIGNATURE

CHEMISTRY

- Paul Bickart
- Diana Darling
- Rich Engler
- Greg Fritz
- Daniel Lin
- Kathy Schechter

*Paul Bickart*

*Kathy Schechter*

ENVIRONMENTAL FATE

- Bob Boethling
- Wen-Hsiung Lee
- Laurence Libelo
- David Lynch
- Andy Mamantov

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- Michael Cimino
- Steve Cragg
- Leonard Keifer
- David Lai
- Jim Murphy
- Deborah Norris
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ENVIRONMENTAL EFFECTS

- Gordon Cash
- Vince Nabholz
- Maggie Wilson

*Gordon Cash*

SAT CHAIR/OTHER

- Rebecca Jones
- Leonard Keifer
- Vince Nabholz
- Jim Kwiat

*Vince Nabholz*